Investigation on the Photovoltaic Performance of Quantum Dot Solar Cells through Self-Consistent Modeling of Transport and Quantum Dot Carrier Dynamics

Investigation on the Photovoltaic Performance of Quantum Dot Solar Cells through Self-Consistent Modeling of Transport and Quantum Dot Carrier Dynamics

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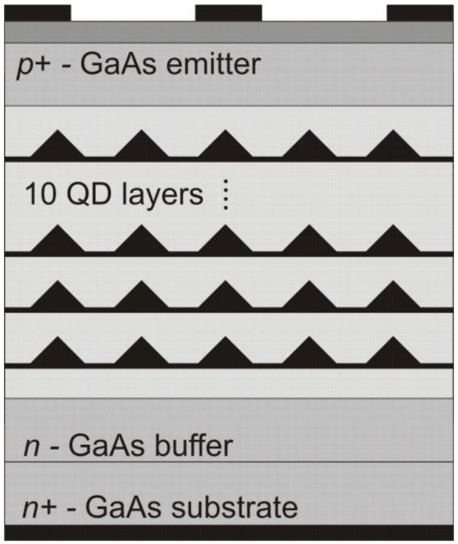
Outline

- Motivation
- Physics-based model coupling transport and carrier dynamics
- Results
  - – Model Validation: case study
  - – Impact of QD *e* and *h* dynamics on J_{sc} and V_{oc}
  - – Modulation doped structures
- Conclusions

III-V Quantum Dots

- Attractive technology to enhance the efficiency of GaAs single- and multi-junction solar cells through bandgap and carrier dynamics engineering
- Possible method for the realization of Intermediate Band solar cells
- The actual potentiality is yet to be assessed

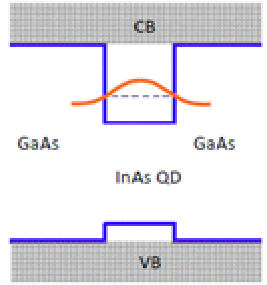
- Underlying physics involves a complex interplay between microscopic and nanoscopic processes → physics-based models are key to understanding the QD role on device performance

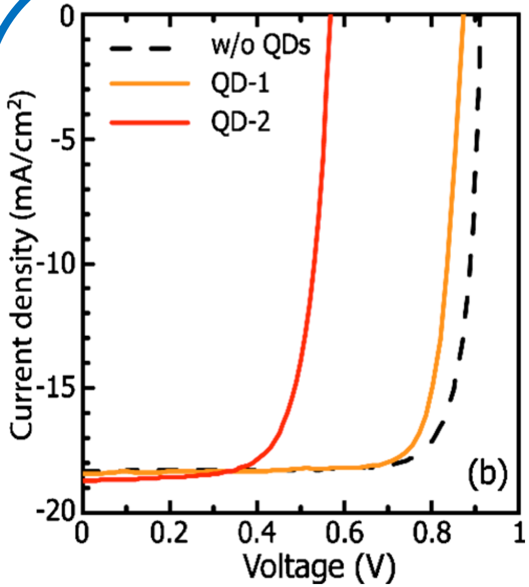


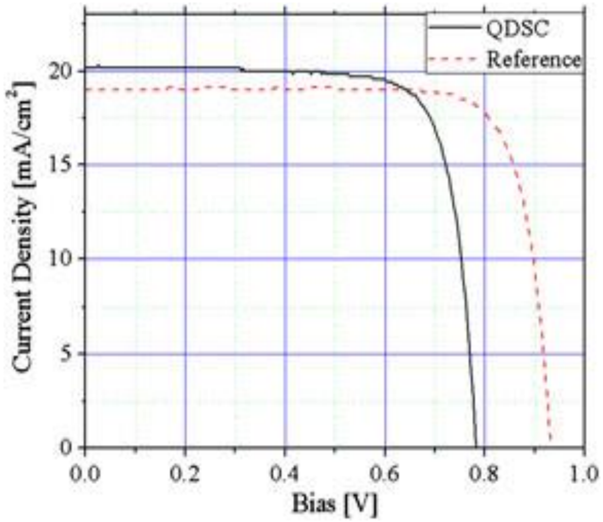
Typical device structure

State of art performance: undoped cells

uncoupled QDs



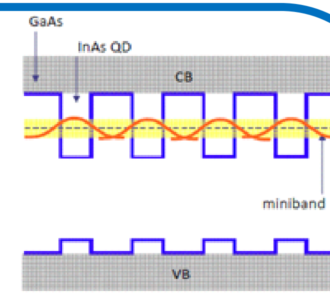


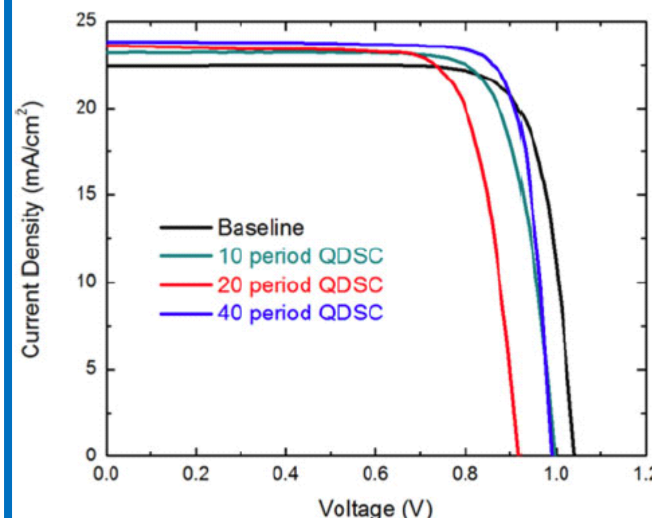


Arakawa's group: Guimard et al. APL, 96, 2010

Jagadish's group: Jolley et al. Prog. Photovolt: Res. Appl. (2012)

QD superlattice

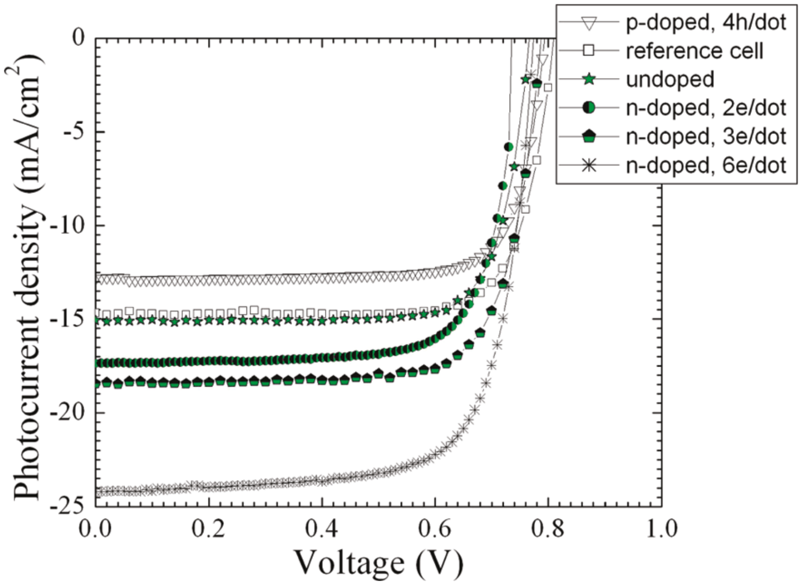




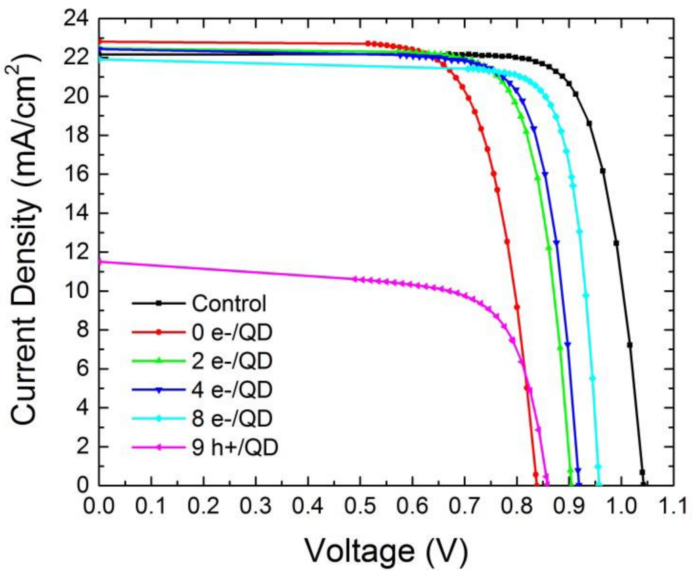
Hubbard's group: Bailey et al., IEEE JPV, Vol.2, pp. 269, 2012

- Small J_{sc} increase, mainly due to WL photogeneration (from EQE measurements)
- V_{oc} degradation
- Room Temperature performance dominated by thermal escape

State of art performance: doped cells



Sablon's group: Sablon et al. Nano Lett, 11, 2011

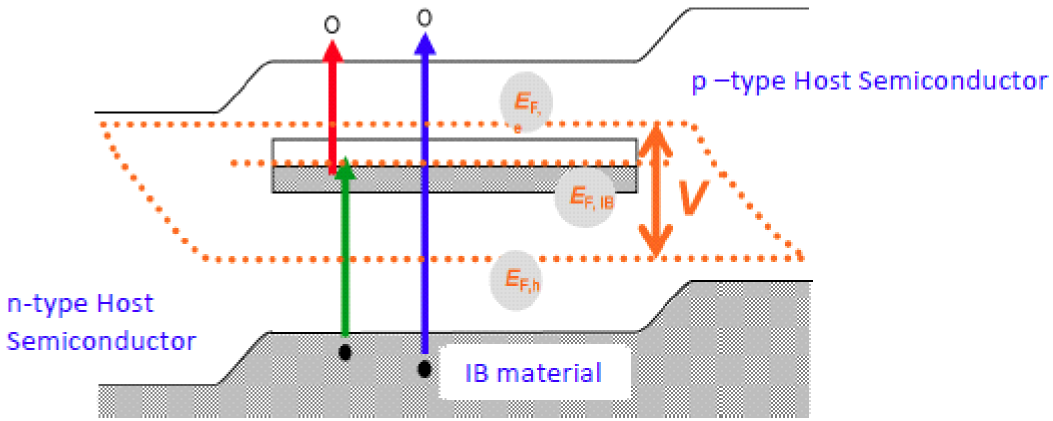


Hubbards's group: to be published in IEEE JPV 2014

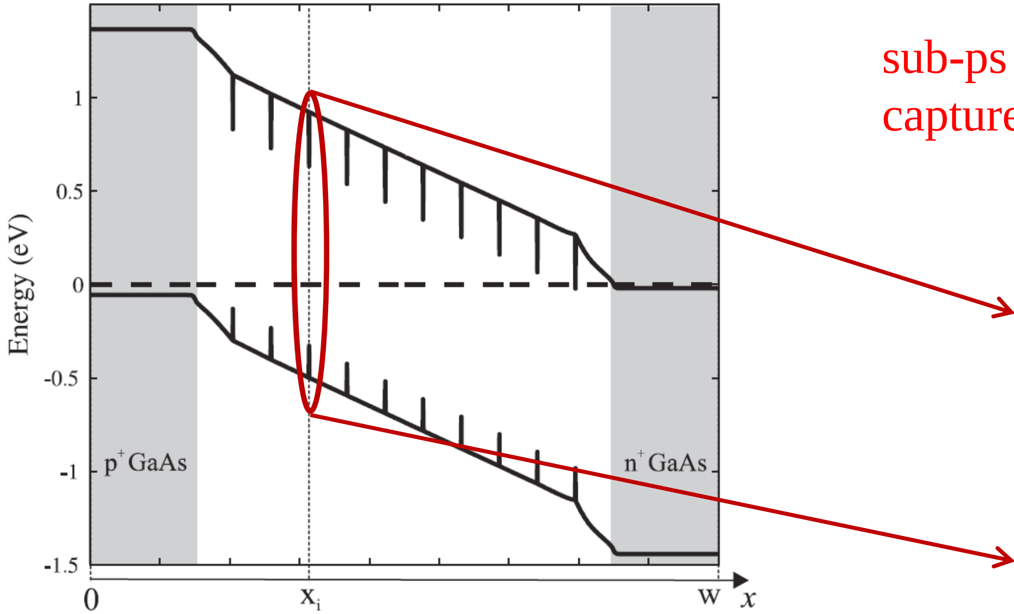
- *n*-doping (d-doping, direct doping) beneficial for V_{oc} recovery
- some results have shown an increase of J_{sc} with *n*-doping, whereas others do not show any significant improvement; p-doping kills J_{sc}
- The effect of doping is thought to modify the dynamics of capture and escape processes in/out the QDs => a model including inter-sub-band carrier dynamics may be useful to get deeper insight

State-of-art modeling approaches

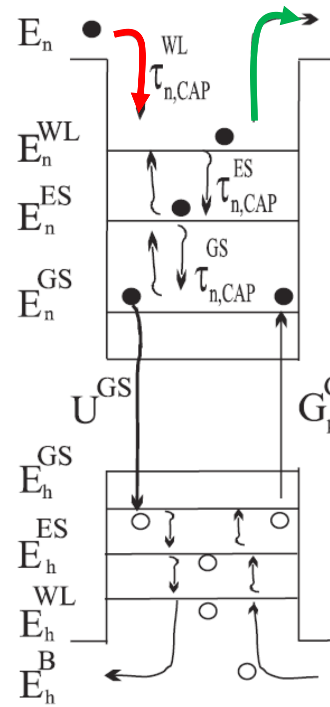
- Most models developed within the IB theory
  - Detailed balance principle, not suitable for device-level analysis
  - Device-level models based on drift diffusion complemented by a discrete energy level associated to the QD array ->
    - does not allow to describe inter-sub-band charge transfer between the QD states
    - suitable only for superlattice structures



This work: drift-diffusion + QD carrier dynamics *



sub-ps B->WL capture



Only thermal escape process at room T

Cascade relaxation through QD state; few ps capture dynamics, several picoseconds escape

Fast sub-ps inter-band hole dynamics due to closer energy states

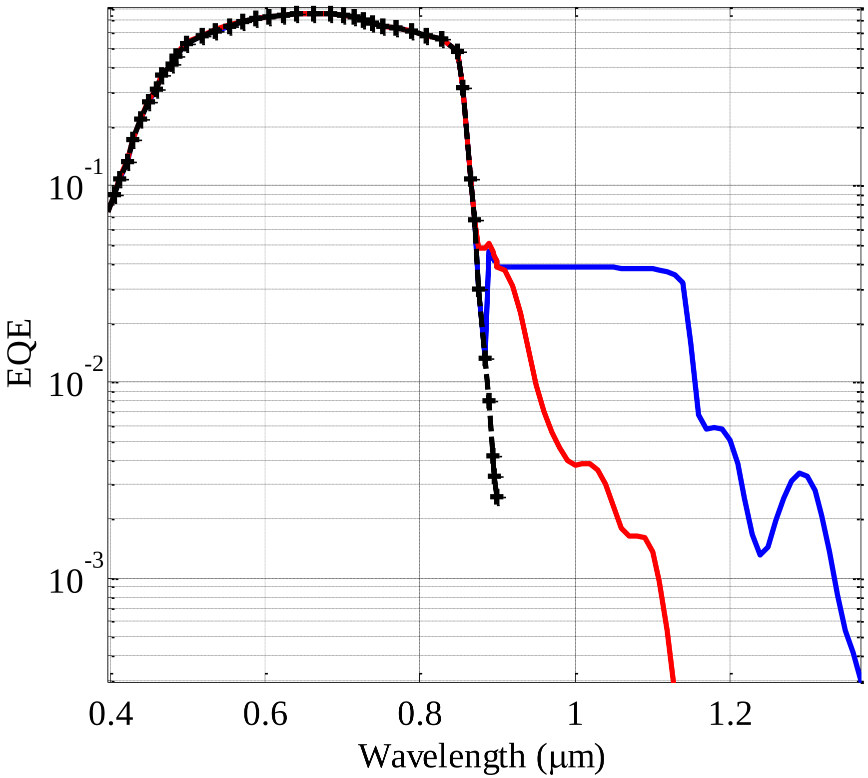
- Tunneling escape from WL → B can be included
- considered only uncoupled QD layers

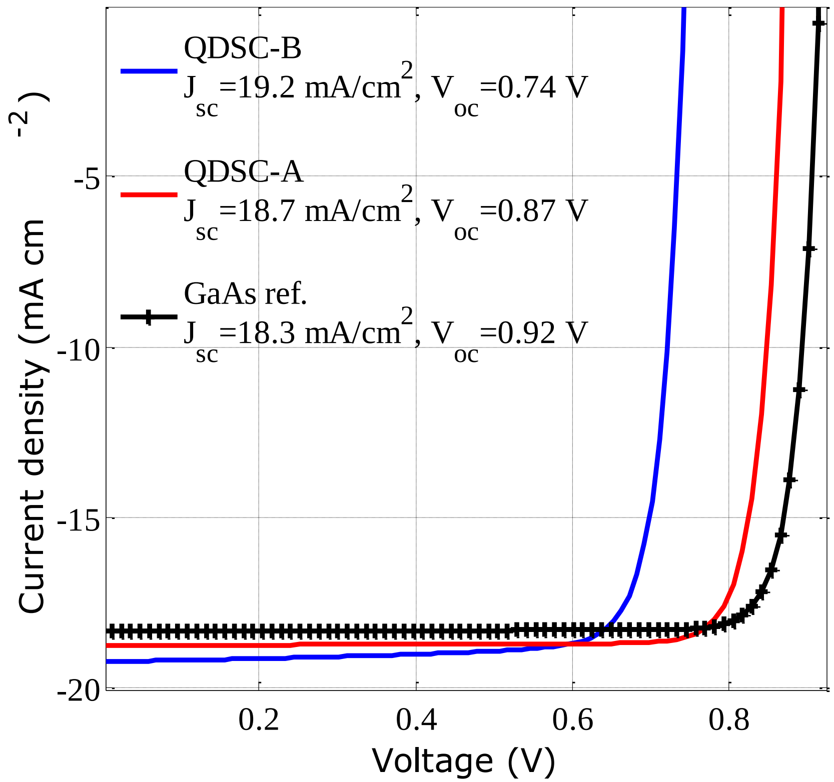
* M. Gioannini et al., IEEE JPV, 2013

Results

- **Model Validation – Case study**
- Impact of QD *e* and *h* dynamics on J_{sc} and V_{oc}
- Modulation doped structures

Case study: correlation between QD size and photovoltaic performance





- ΔJ_{sc} with respect to ref cell ~ integrated QD's photogeneration rate: almost full collection efficiency
- Voc degradation larger for the larger QDs, i.e. with higher B-WL barrier

Results

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- **Impact of QD *e* and *h* dynamics on J_{sc} and V_{oc}**
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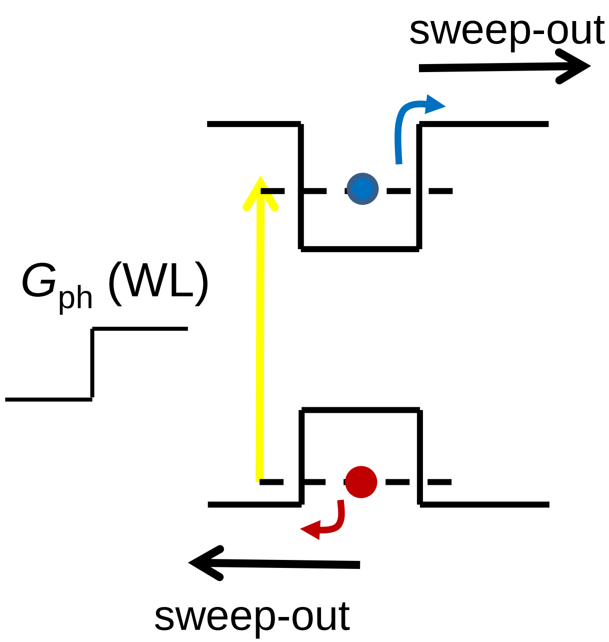
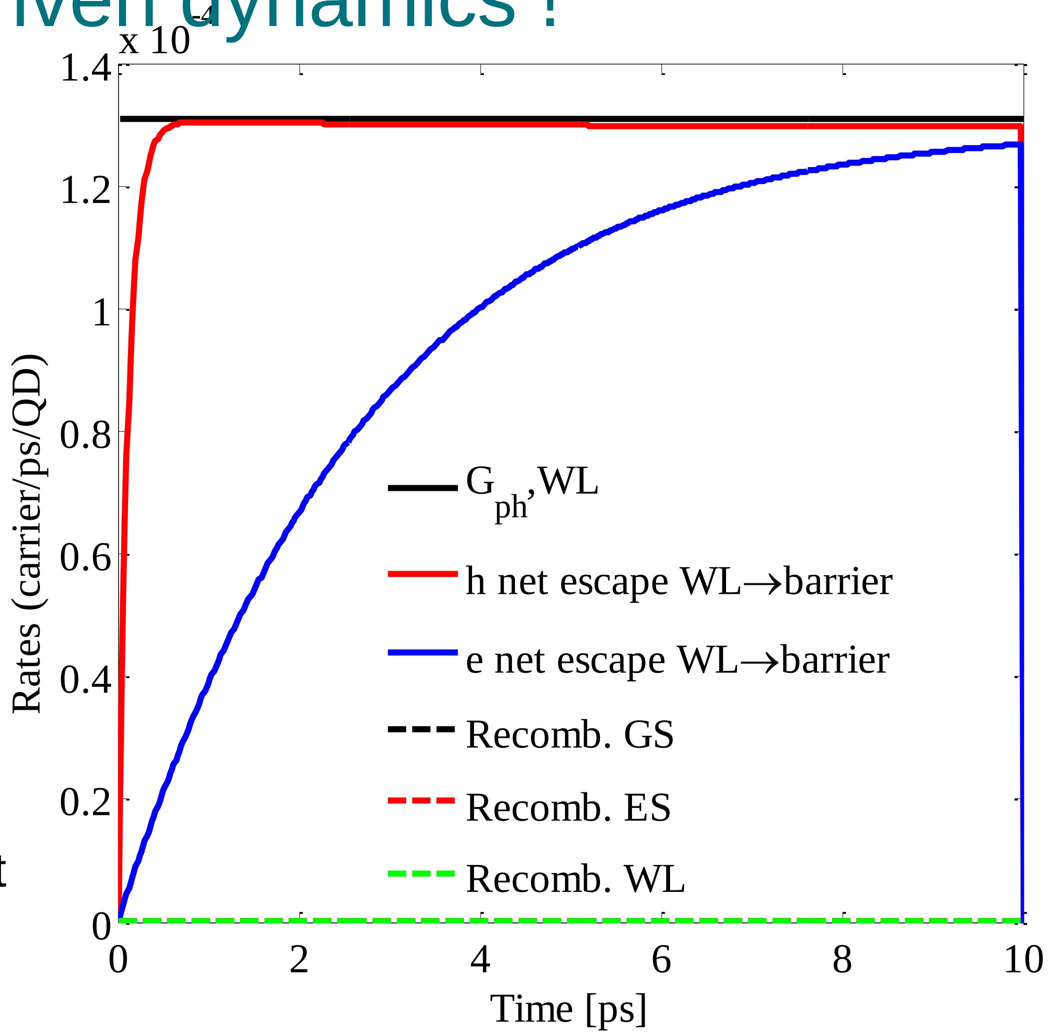
High collection efficiency despite slow electron dynamics → hole-driven dynamics !





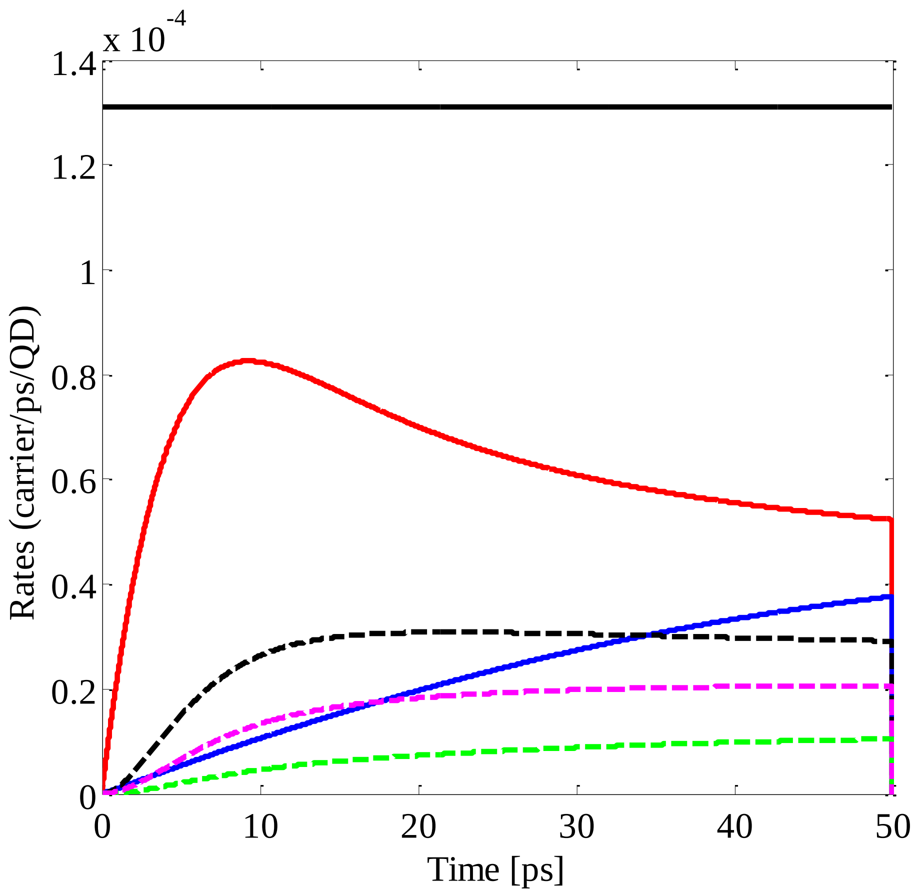
@ short circuit: high field → short sweep-out time in the Barrier

Escape/sweep-out "bottleneck" → V_{oc} degradation

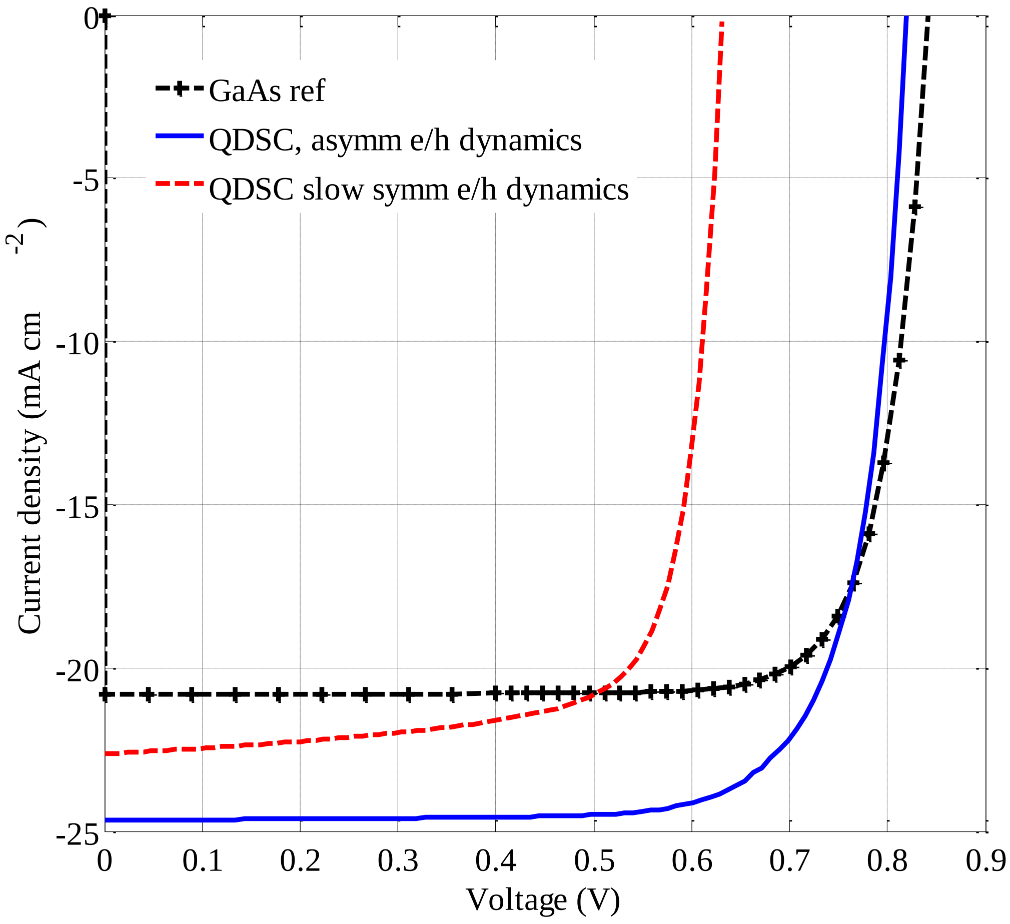
- Under forward bias: lower electric field → higher
- barrier sweep-out time

- Capture/recombination becomes dominant over escape/sweep-out

- Effect as stronger as (higher) lower is the individual e/h (capture) escape

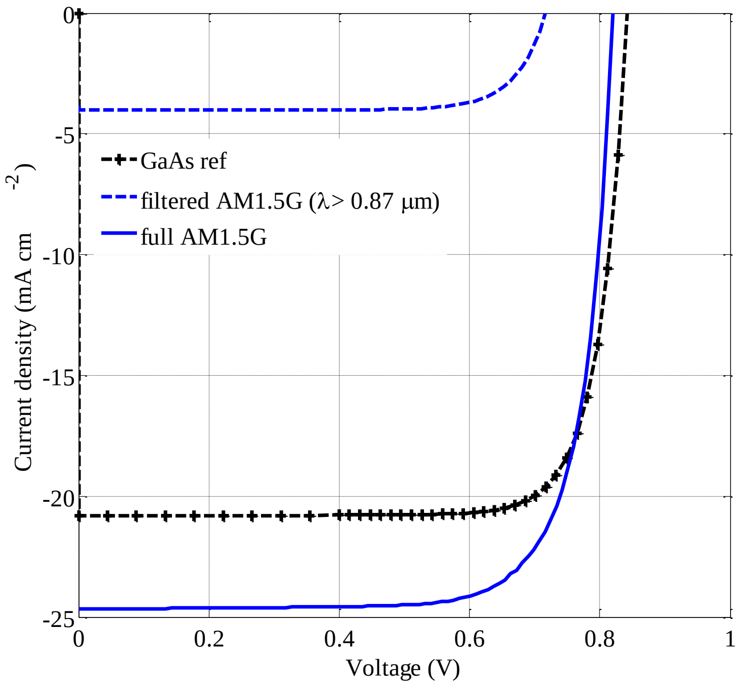


More on effect of e/h dynamics: “excitonic-like” case

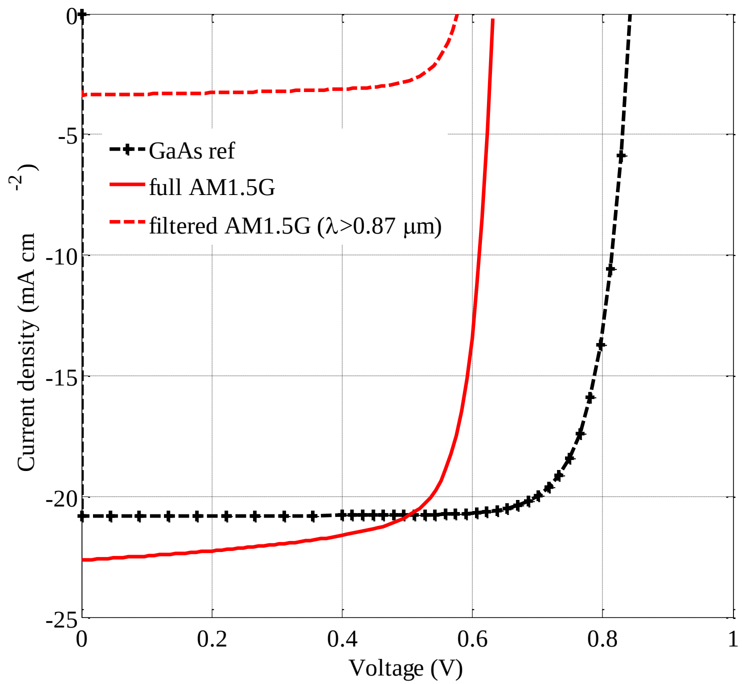


QD contribution to J_{sc} *vs.* e/h dynamics

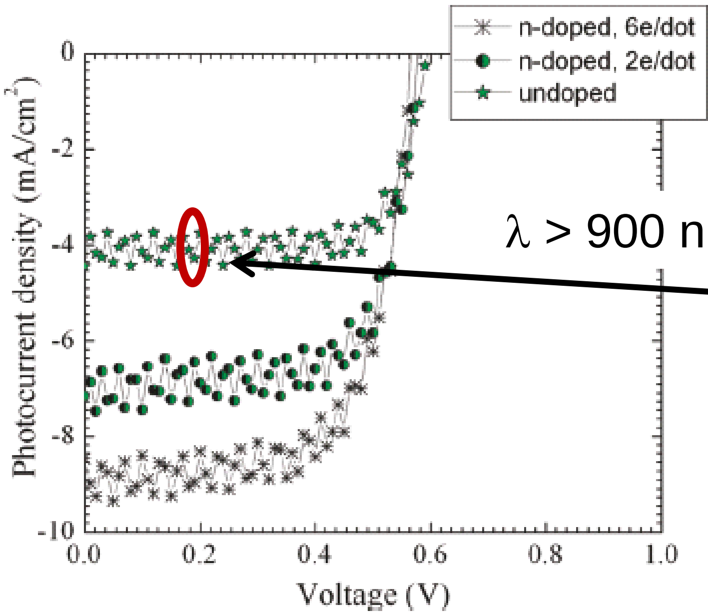
hole dynamics much faster than electrons
→ linear (additive) behavior



"excitonic-like" case
→ NON linear behavior

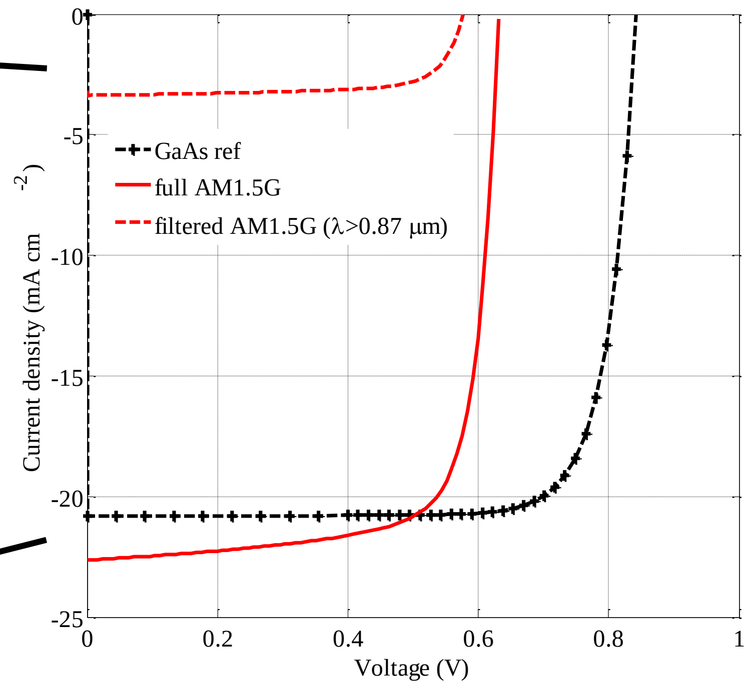


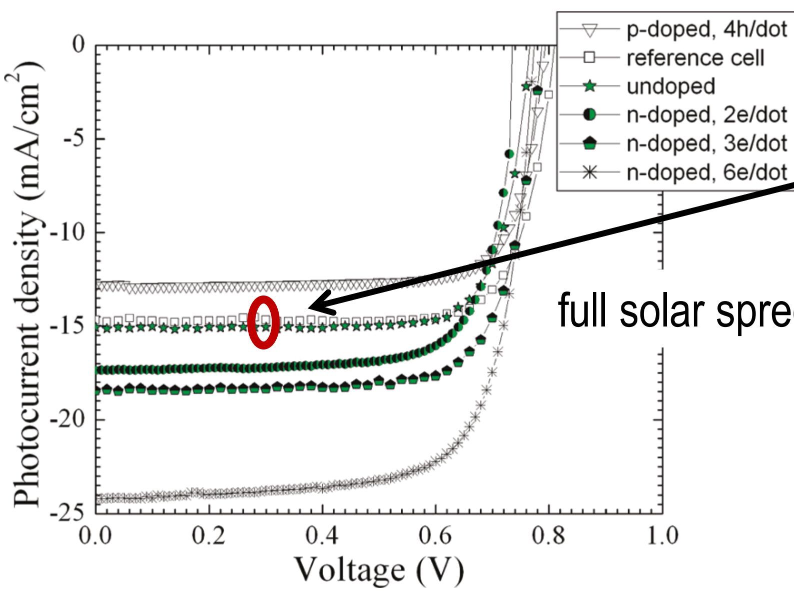
QD contribution to J_{sc} *vs.* e/h dynamics



λ > 900 nm

“excitonic-like” case
→ NON linear behavior

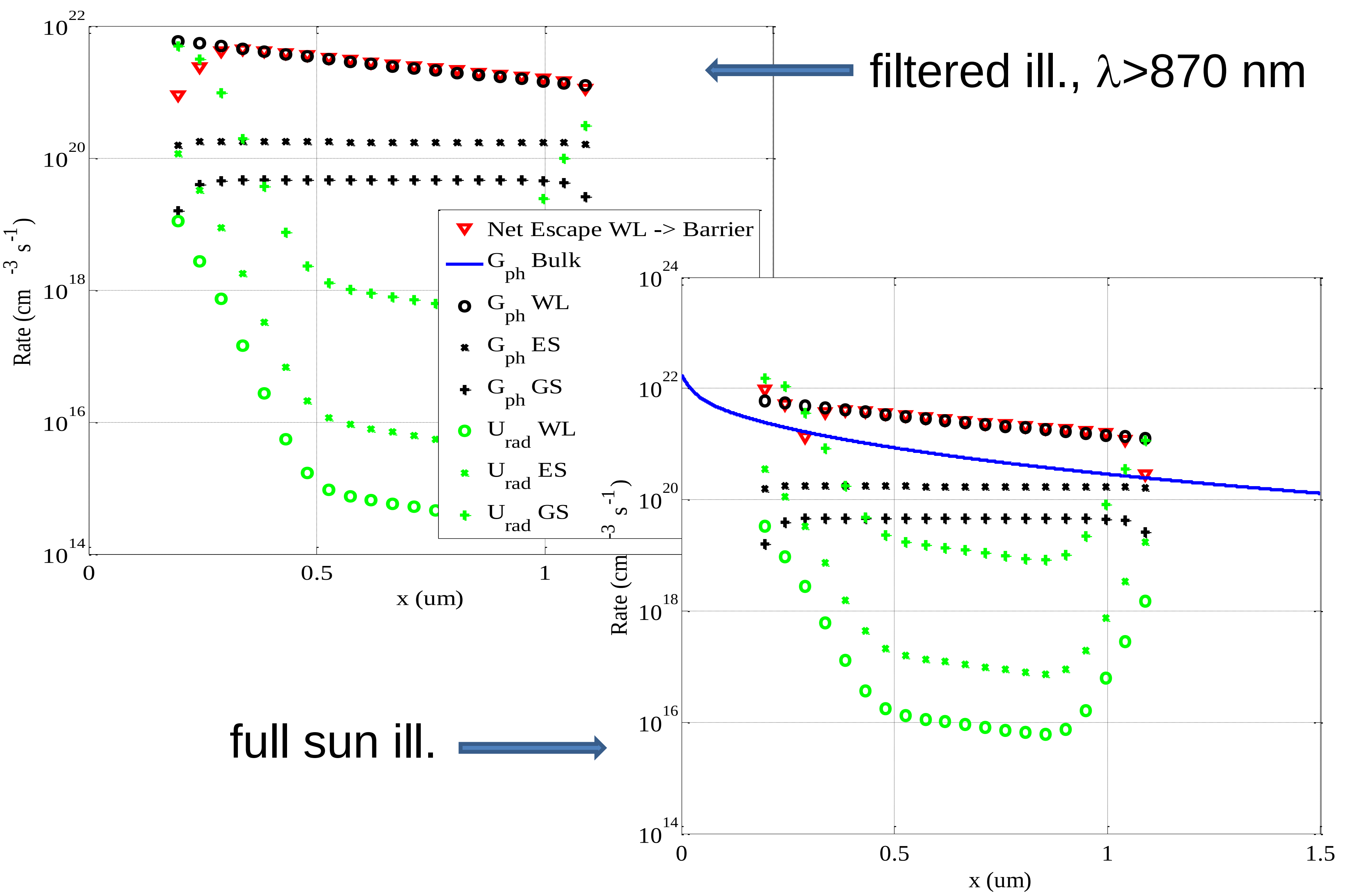




full solar sprectrum

Sablon’s group: Sablon et al. Nano Lett, 11, 2011

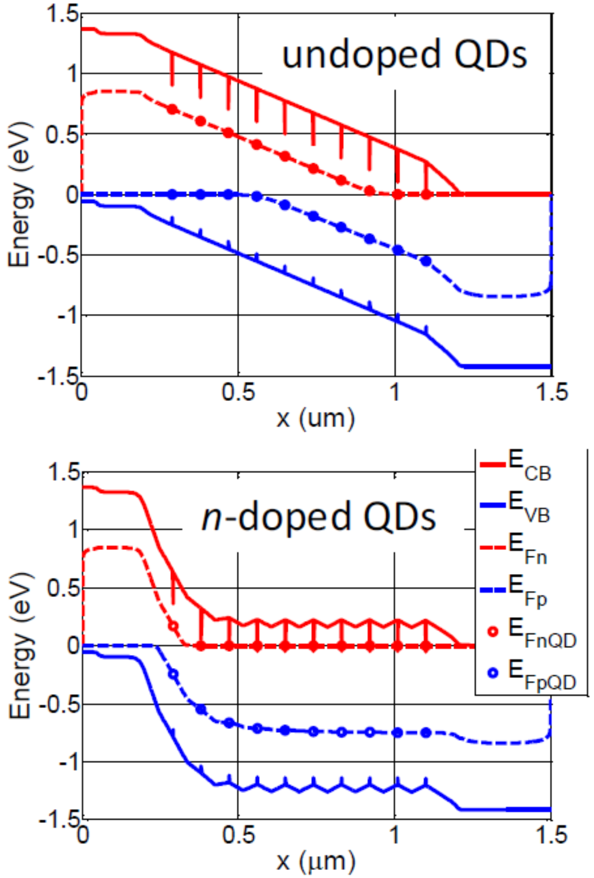
Rates under full & filtered illumination

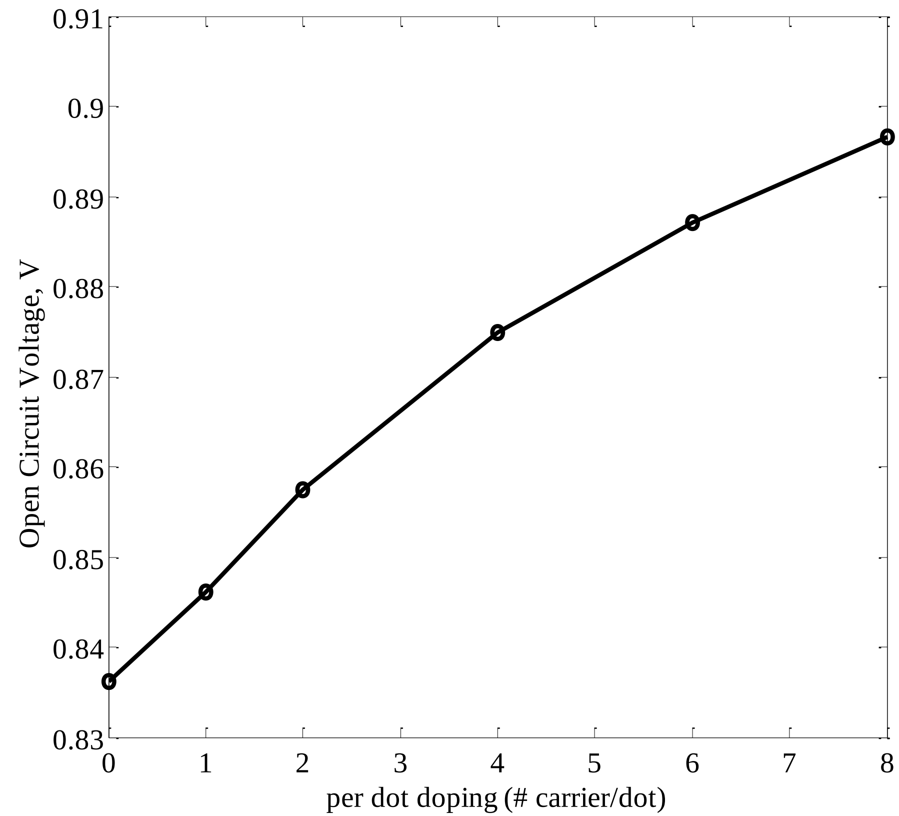


Results

- Model Validation – Case study
- Impact of QD *e* and *h* dynamics on J_{sc} and V_{oc}
- **Modulation doped structures**

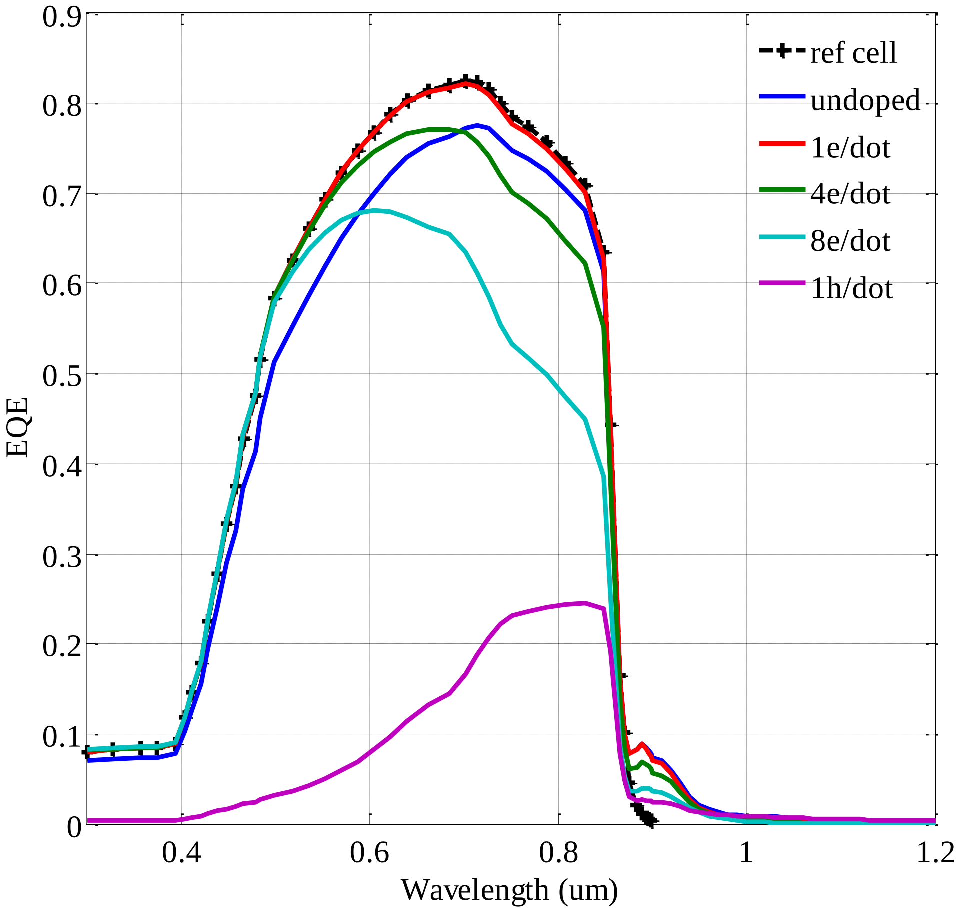
Modulation doping structures: V_{oc} recovery in *n*-doped samples

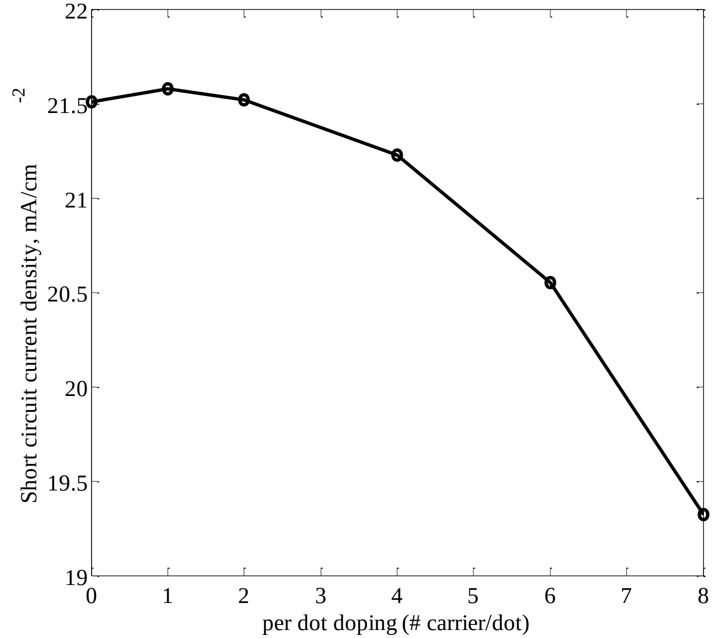


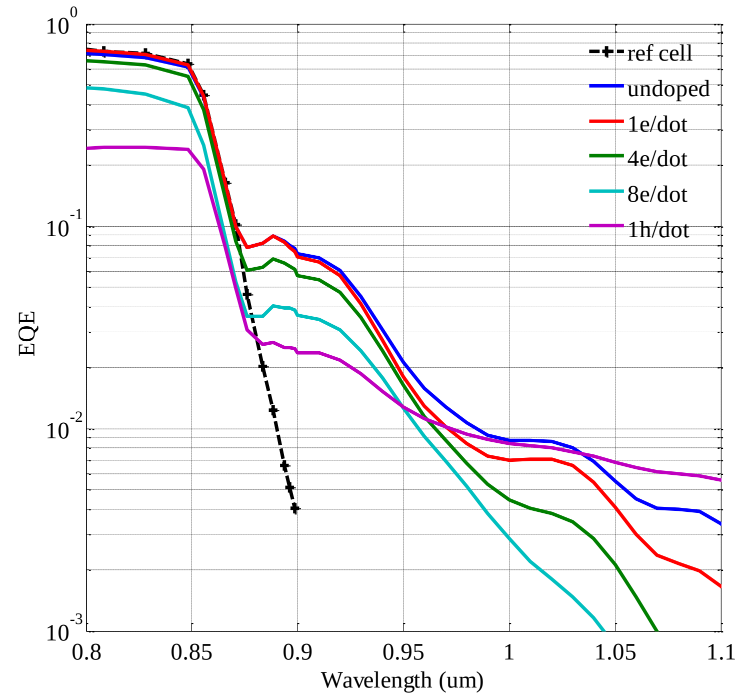


- Dominant effect is suppressed electron capture from QDs
- Simulated Voc recovery ~ 70 mV for 8e/dot; p-doping quite ininfluent
- Experiments: 121 mV for 8e/dot δ-doping (Polly at al., to appear in JPV 2014); 105 mV for 18e/dot direct doping (Lam et al., NanoEnergy 2014,)

Modulation doping structures: J_{sc} and EQE







Conclusions

- Developed a device-level model including QD intersubband carrier dynamics and transport
- Simulated results in good agreement with typical experimental performance
- Highlighted impact of e/h individual dynamics and de-synchronization on apparent sub-bandgap collection efficiency and Voc degradation
- Preliminary analysis of modulation doped structures

Coupled drift-diffusion / QD model

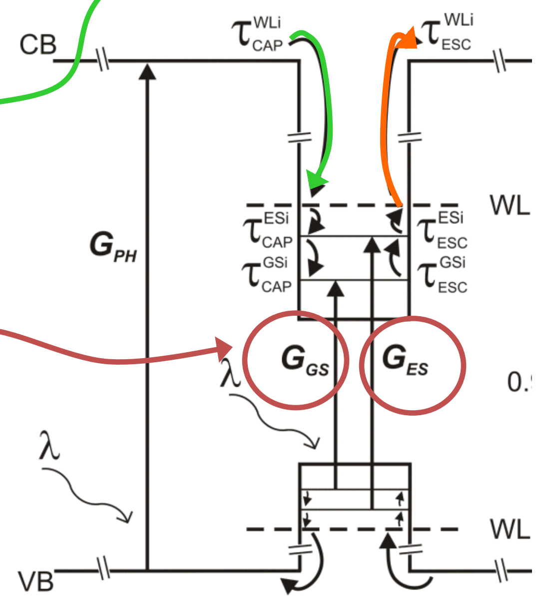
$$\frac{\partial E}{\partial x} = \frac{q}{\varepsilon}\left(p - n + N_d^+ - N_a^- + p_{WL_i} - n_{WL_i} + p_{ES_i} - n_{ES_i} + p_{GS_i} - n_{GS_i}\right)$$

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x}\left(\mu_n n E + D_n \frac{\partial n}{\partial x}\right) - R_{TOT} + G_{PH} - R_{N\,CAP}^{\,B\rightarrow WL} + R_{N\,ESC}^{\,WL\rightarrow B}$$

Photo-generation in the barrier

Capture from the barrier in the QDs

Photo-generation of carriers in the QDs



Escape of photo-generated carriers from the QDs to the barrier

QD Rate Equations

Recombination

$$\frac{\partial n_{WL_i}}{\partial t} = \frac{n}{\tau_{nCAP}^{WL_i}} - \frac{n_{WL_i}}{\tau_{nESC}^{WL_i}} - \frac{n_{WL_i}}{\tau_{nCAP}^{ES_i}}\left(1 - \frac{n_{ES_i}}{N_D \mu_{ES}}\right) + \frac{n_{ES_i}}{\tau_{nESC}^{ES_i}} + G_{PH_{WL}}$$

$$\frac{\partial n_{ES_i}}{\partial t} = \frac{n_{WL_i}}{\tau_{nCAP}^{ES_i}}\left(1 - \frac{n_{ES_i}}{N_D \mu_{ES}}\right) - \frac{n_{ES_i}}{\tau_{nESC}^{ES_i}} - \frac{n_{ES_i}}{\tau_{nCAP}^{GS_i}}\left(1 - \frac{n_{GS_i}}{N_D \mu_{GS}}\right) + \frac{n_{GS_i}}{\tau_{nESC}^{GS_i}}\left(1 - \frac{n_{ES_i}}{N_D \mu_{ES}}\right) - \frac{N_D}{\tau_{REC}^{ES_i}} \frac{n_{ES_i}}{N_D \mu_{ES}} \frac{p_{ES_i}}{N_D \mu_{ES}} + G_{PHES_i}$$

$$\frac{\partial n_{GS_i}}{\partial t} = \frac{n_{ES_i}}{\tau_{nCAP}^{GS_i}}\left(1 - \frac{n_{GS_i}}{N_D \mu_{GS}}\right) - \frac{n_{GS_i}}{\tau_{nESC}^{GS_i}}\left(1 - \frac{n_{ES_i}}{N_D \mu_{ES}}\right) - \frac{N_D}{\tau_{REC}^{GS_i}} \frac{n_{GS_i}}{N_D \mu_{GS}} \frac{p_{GS_i}}{N_D \mu_{GS}} + G_{PHGS_i}$$

$$G_{PHWL}(x,\lambda) = \int_\lambda \alpha_{WL}(\lambda)\cdot \Phi_{AM1.5G}(\lambda)\cdot \exp(-\alpha_{WL}(\lambda)\cdot x)\cdot d\lambda$$

$$G_{PHES_i}(x,\lambda) = \int_\lambda \alpha_{ES}(\lambda, f_{e_i}, f_{h_i})\cdot \Phi_{AM1.5G}(\lambda)\cdot \exp(-\alpha_{ES}(\lambda, f_{e_i}, f_{h_i})\cdot x)\cdot d\lambda$$

$$G_{PHGS_i}(x,\lambda) = \int_\lambda \alpha_{GS}(\lambda, f_{e_i}, f_{h_i})\cdot \Phi_{AM1.5G}(\lambda)\cdot \exp(-\alpha_{GS}(\lambda, f_{e_i}, f_{h_i})\cdot x)\cdot d\lambda$$

Photo-generation in the QDs states

Redistribution among states